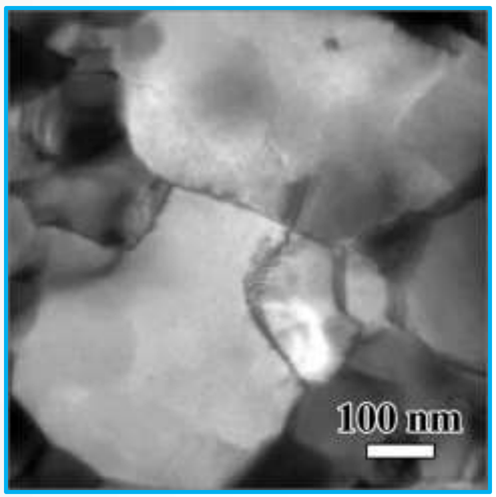
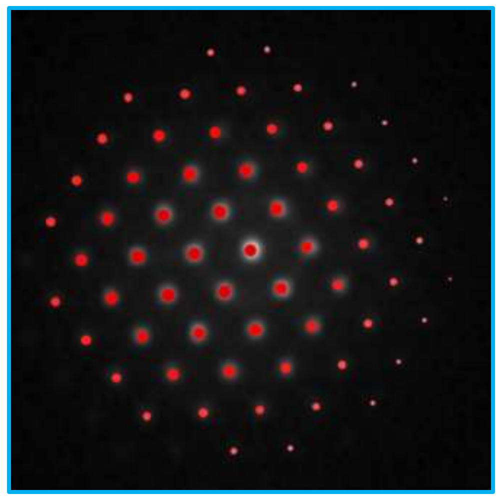
Sandia National Laboratories

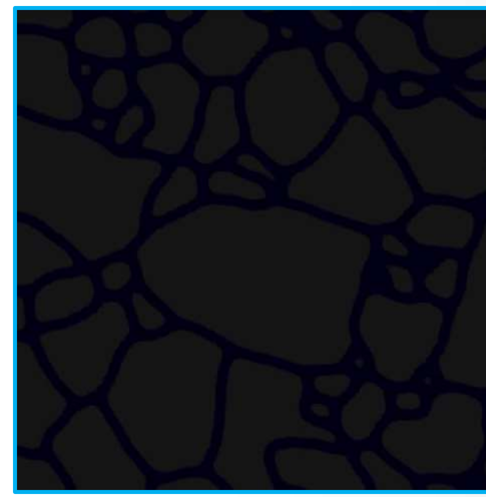
TMS 2016
145th Annual Meeting & Exhibition

SAND2016-1477C

In Situ Characterization and Phase Field Modeling of Irradiation-Induced Grain Growth







Daniel C. Bufford, Fadi F. Abdeljawad, Stephen M. Foiles, and Khalid Hattar
Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY   NNSA National Nuclear Security Administration

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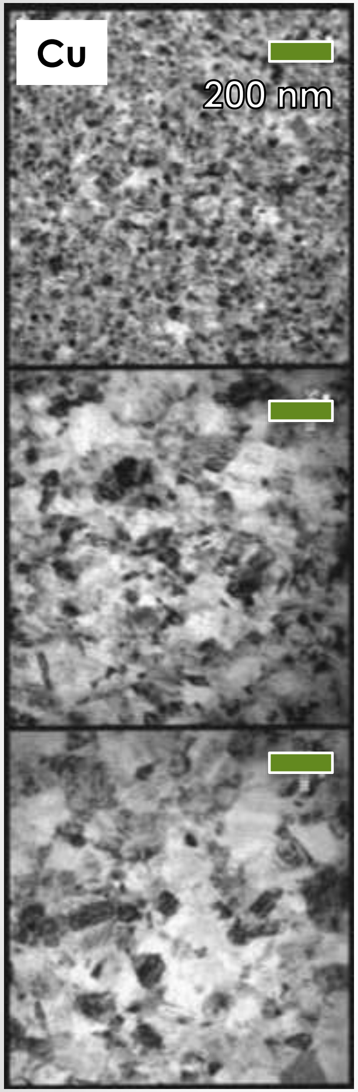
18 February 2016

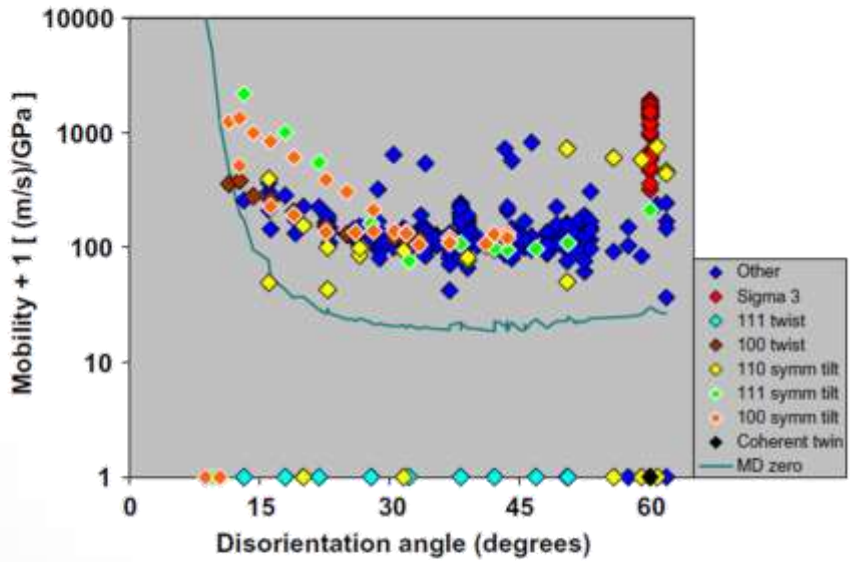
Motivation



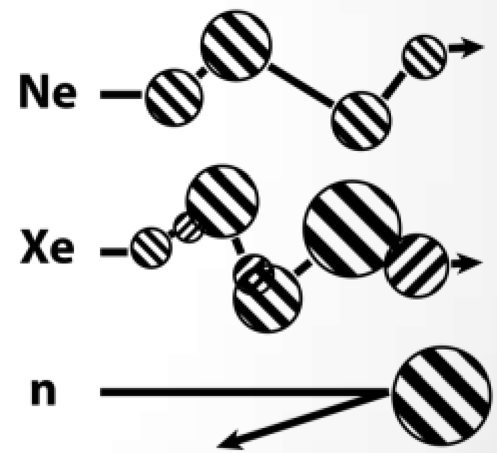
Kaoumi, *et al*, J ASTM Intl, 2006.

Nanocrystalline metals:

- Exemplary mechanical properties.
- Abundant sinks for structural and chemical defects.
- Ideal candidates for radiation-tolerant materials?



Olmstead, *et al*, Acta Mater, 2009.



Schematic recoil spectra for 1 MeV particles in Cu. Sizes represent recoil energies. After Averback, J Nucl Mater, 1994.

What are the relationships among ion damage, grain boundary character, and grain growth?

Sandia's *In situ* Ion Irradiation TEM (I^3TEM)

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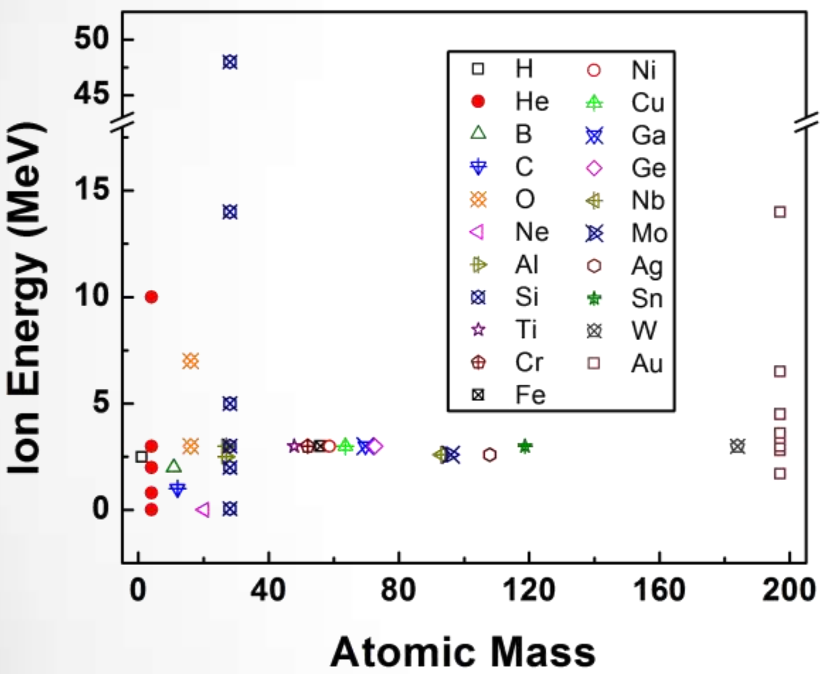
Collaborator: D.L. Buller

10 kV Colutron - 200 kV TEM - 6 MV Tandem



Hattar, *et al*, Nucl Instr Meth Phys Res B, 2014.

Enables real-time studies of samples under irradiation.

Synergistic *In Situ* Capabilities

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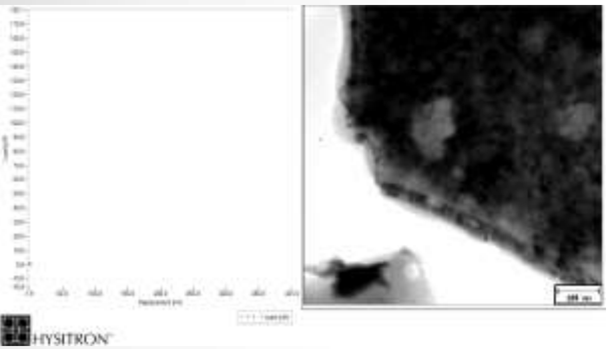
Mechanical



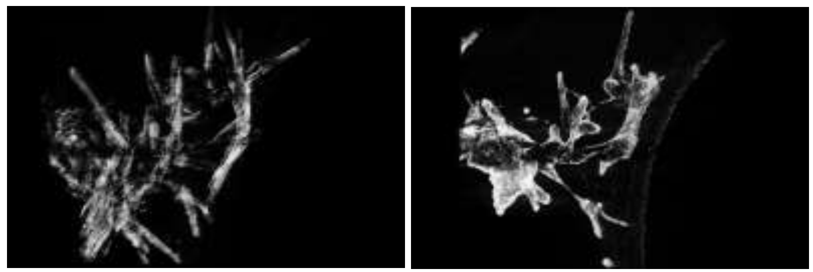
Hysitron PI95 TEM Picoindenter
Gatan 654 Straining Holder
Direct correlation of dose and defect density with resulting changes in strength, ductility, and defect mobility

Environmental

Protochips Liquid and Gas Flow
Effects of radiation on corrosion and gas loading at the grain level

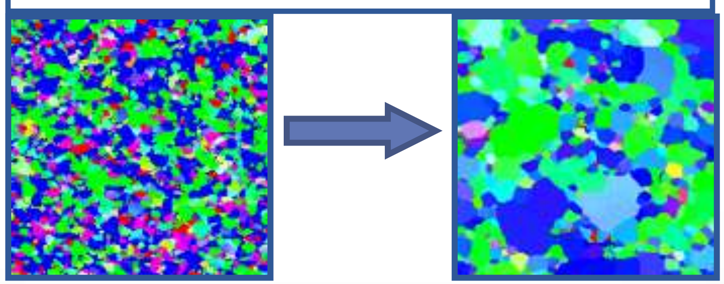
Structural

Hummingbird Tomography Stage
Gatan 925 Double Tilt Rotate
Morphology changes as a result of radiation damage



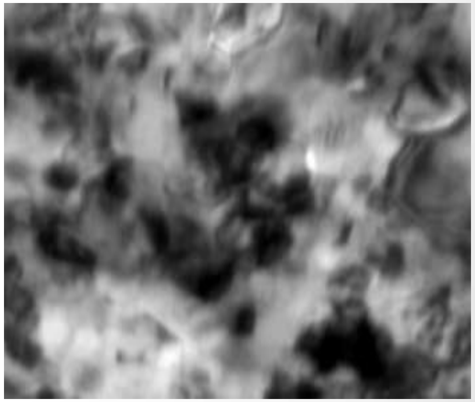
Texture

Nanomegas ASTAR
Quantifying orientation changes as a result of radiation, implantation, and heat.



Thermal

Hummingbird Heating Stage
Coupling effects of temperature and irradiation on microstructural evolution up to 800 °C



The application of advanced microscopy techniques to characterize synergistic effects in a variety of extreme environments

In Situ Irradiation

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- Au foil during bombardment with 10 MeV Si^{3+}
- ~22 s of 4000s total experiment time

2× real time

Locations of single ion strikes and resulting microstructural change captured.

Quantification: Overall

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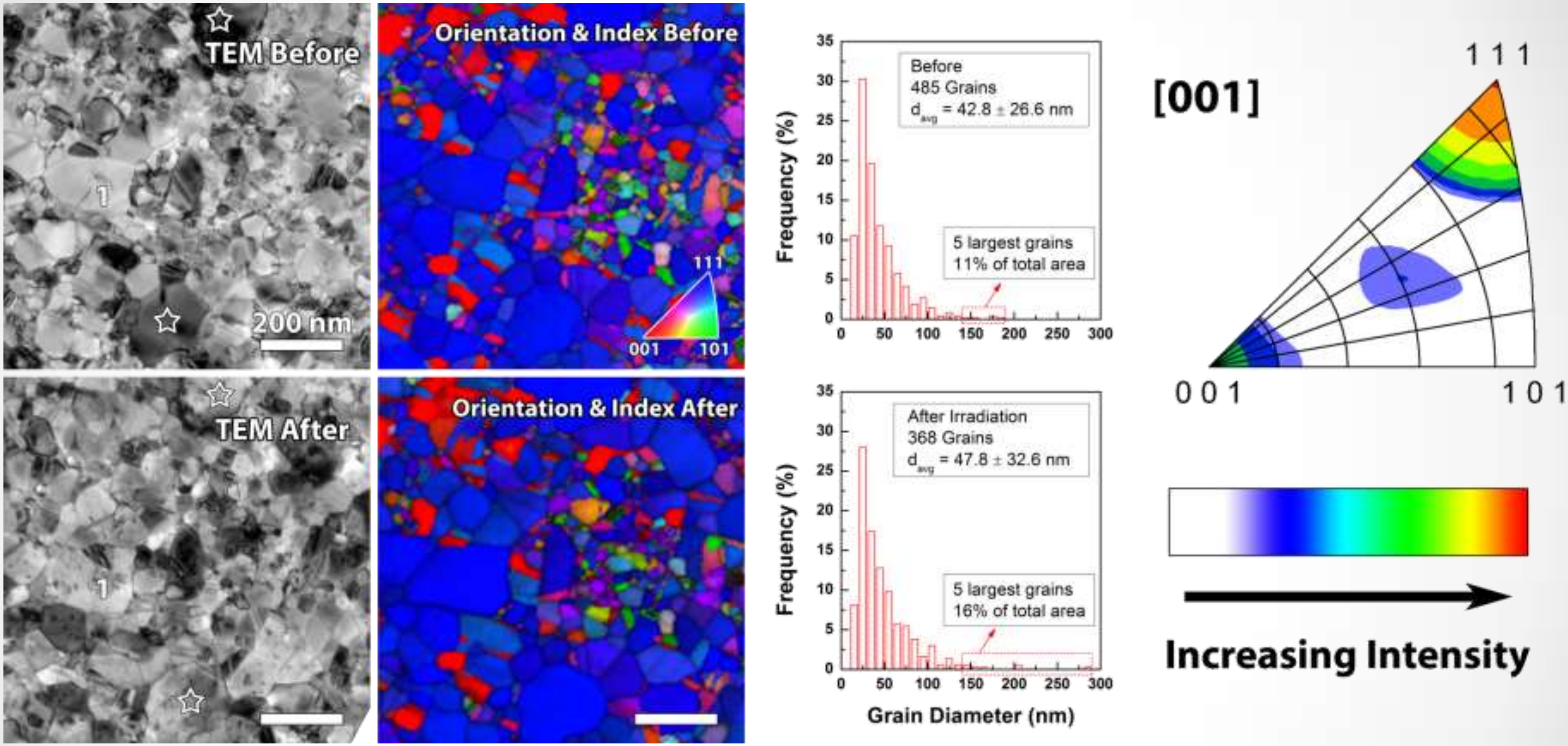
Bufford, *et al*, J Appl Phys, 2015.

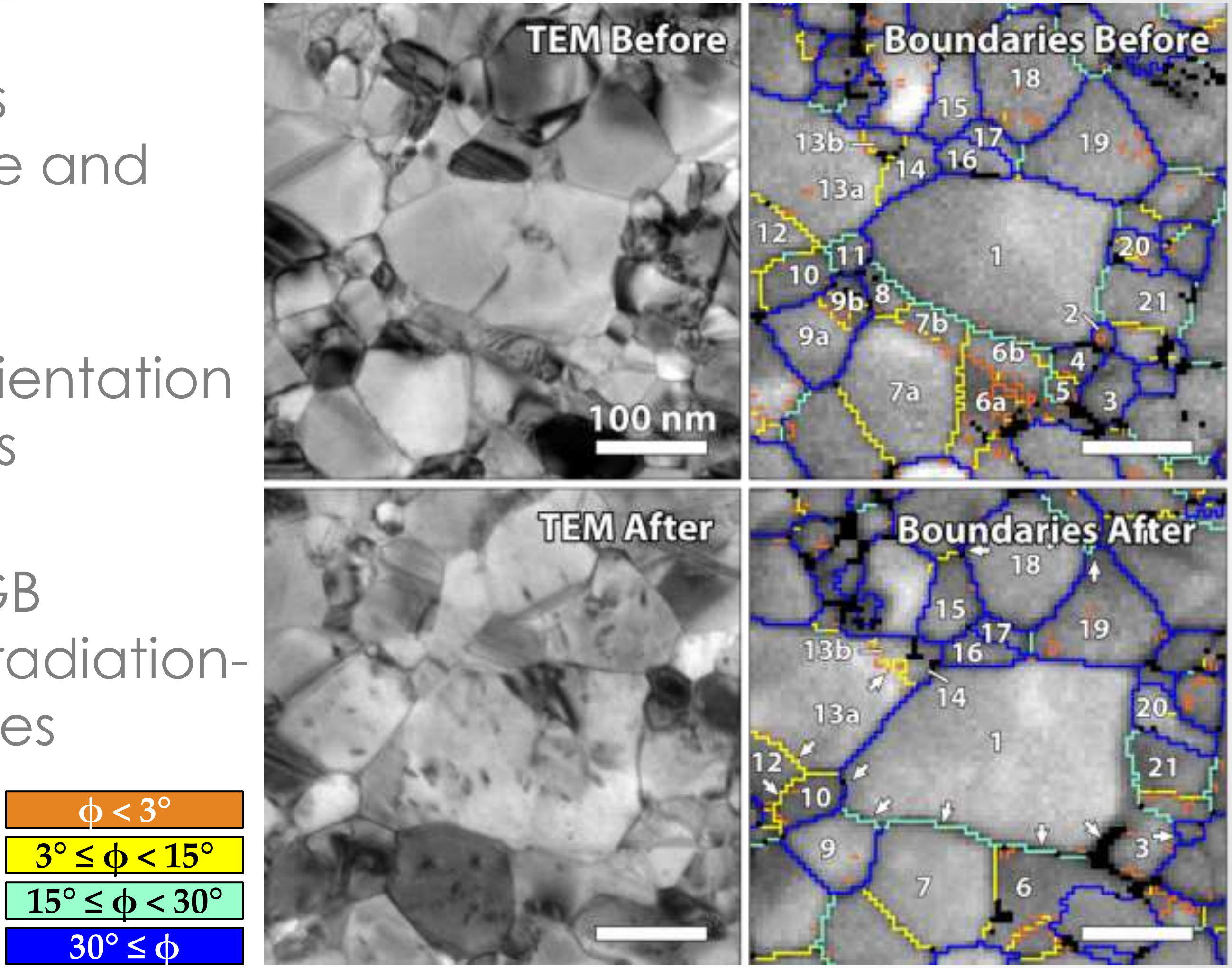


- Same area characterized before and after irradiation.
  - Local grain size, orientation, boundary character
  - Hundreds of grains counted in minutes

Rapid quantification of statistically relevant numbers of grains and boundaries.

Quantification: Local

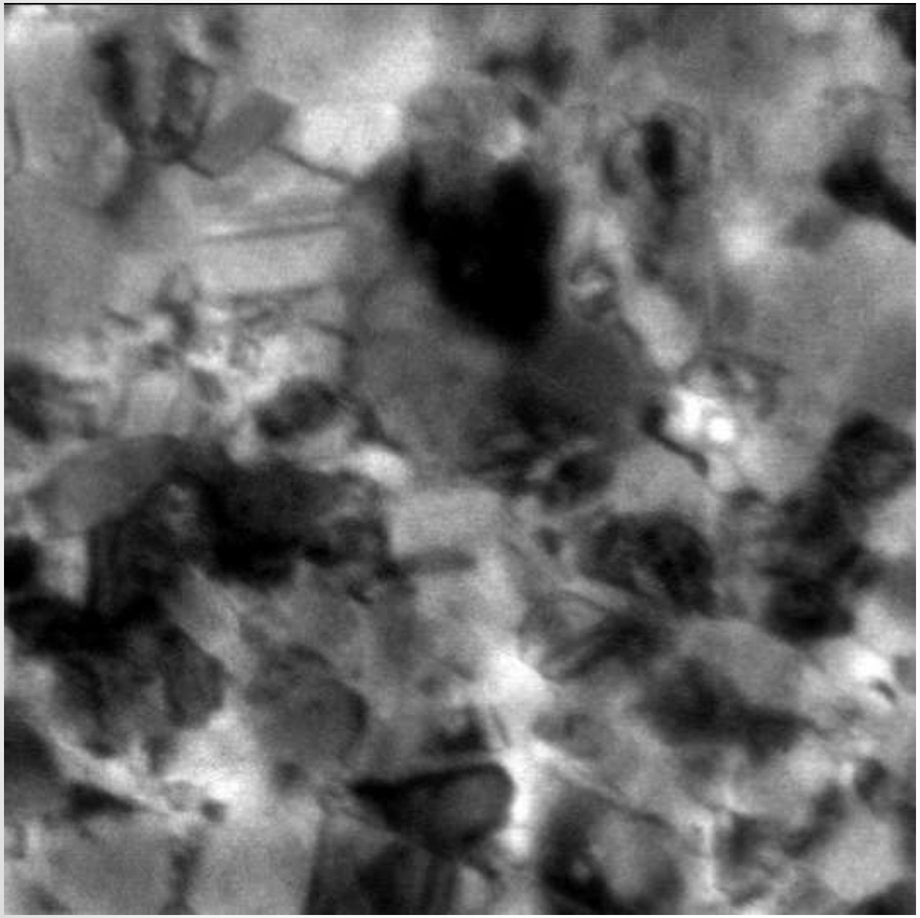
- The same grains identified before and after irradiation
- Individual grain boundary misorientation angles and axes quantified
- Correlation of GB properties and radiation-induced changes

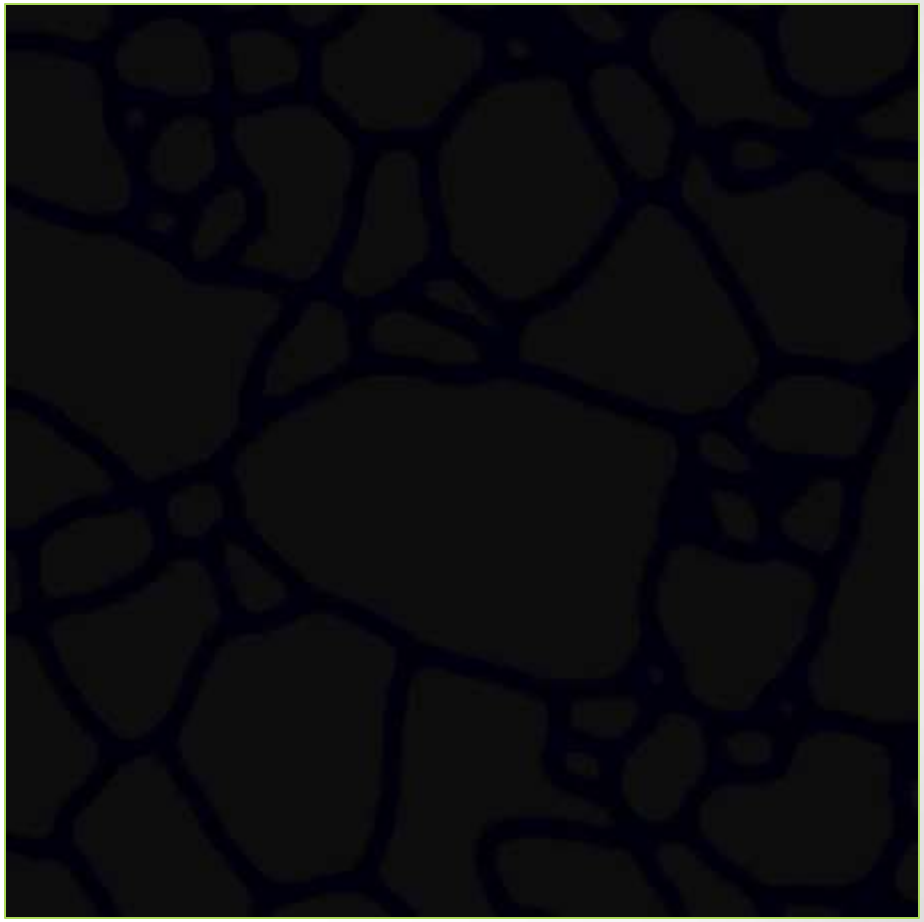


Bufford, *et al*, J Appl Phys, 2015.

Grain boundary misorientation angle and axes quantified

Simulated Irradiation





2× real time

Exp. & Model Comparison

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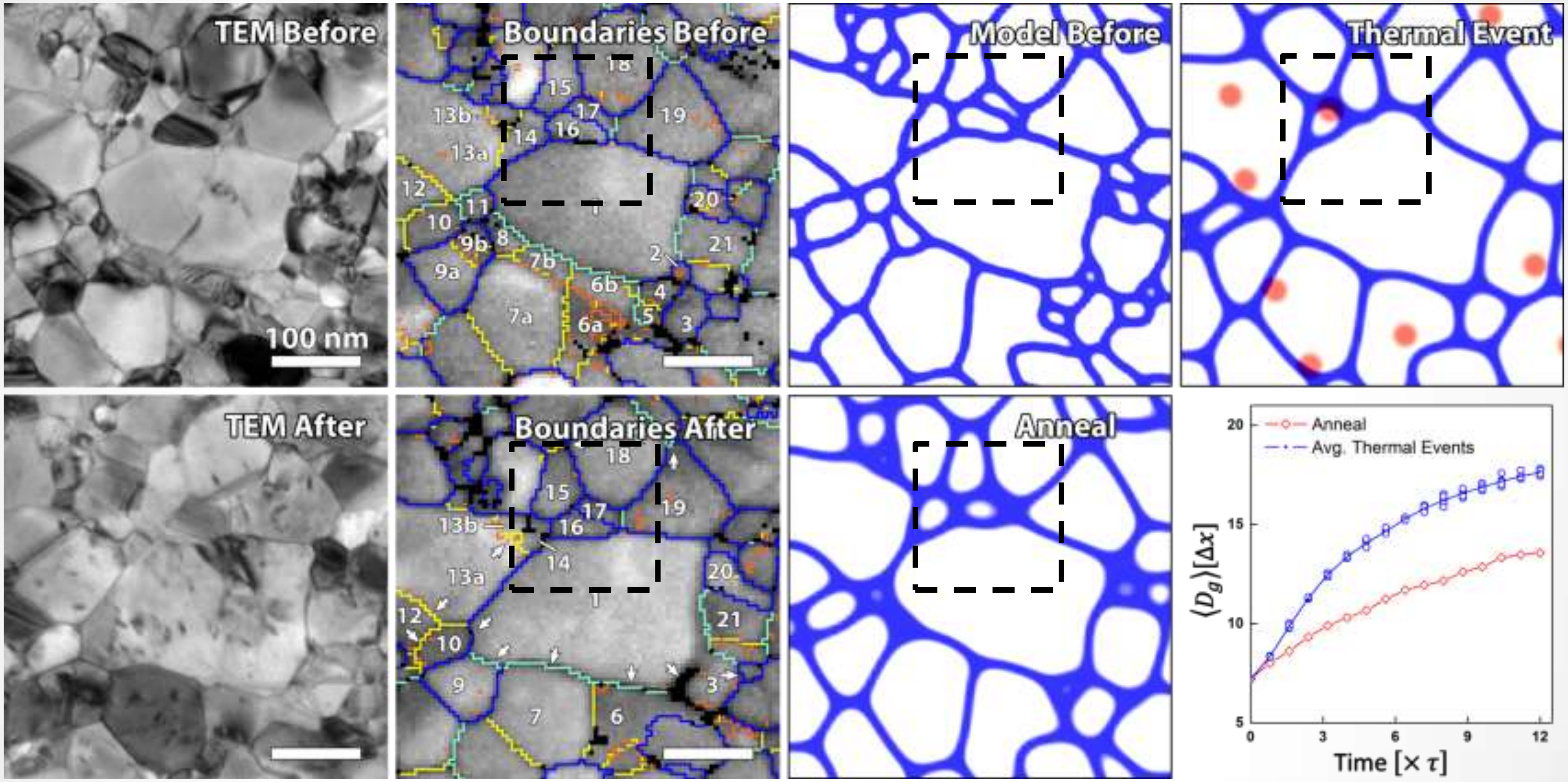
Bufford, *et al*, J Appl Phys, 2015.



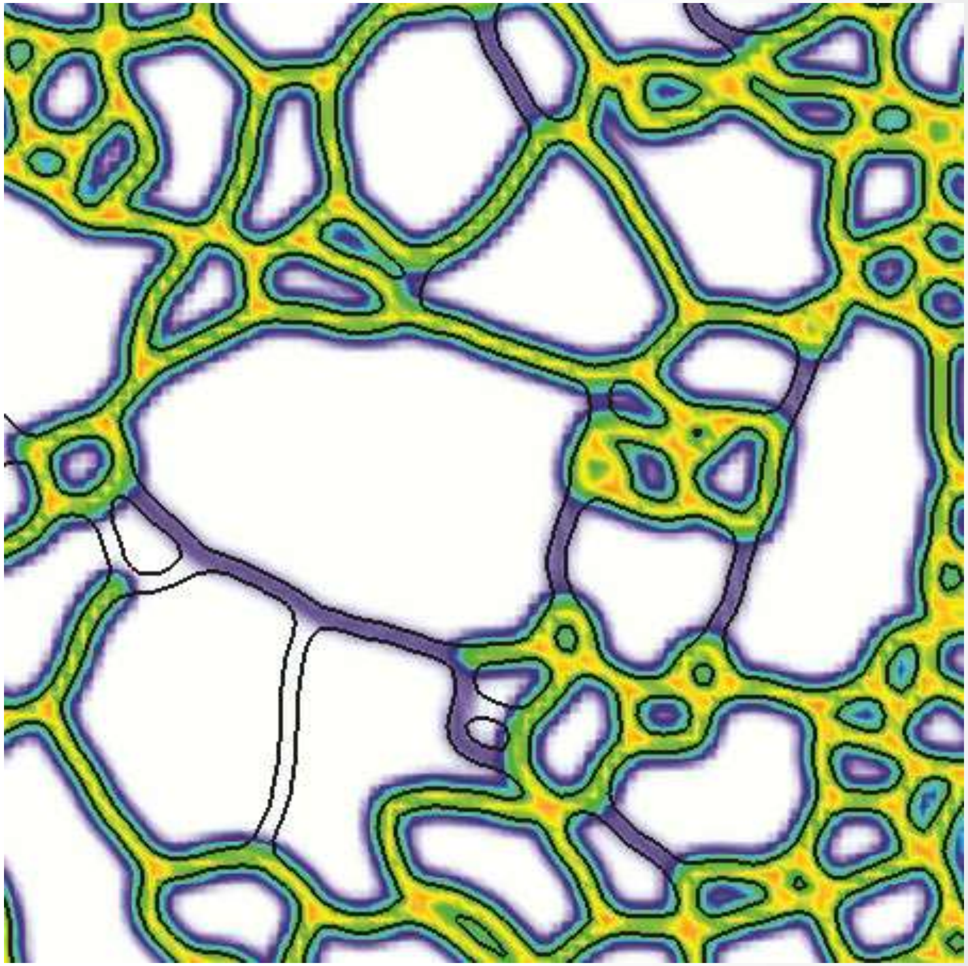
- Overall scaling laws appear consistent
- Subtle deviations from homogenous grain growth

Immobile boundaries suggest importance of non-thermally activated mobility

Model Improvements

- Grain boundary mobility dependent on φ
  - Step function

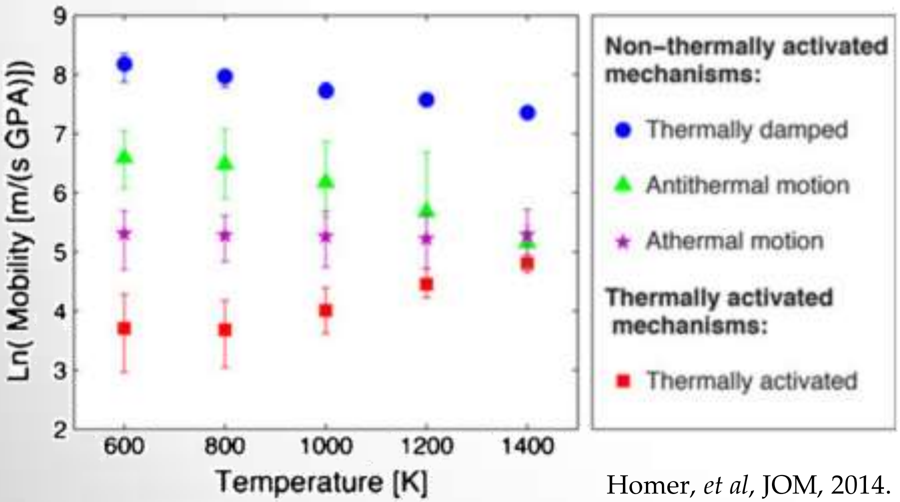
$3° \leq \phi < 15°$ - $M = 0.01$
$15° \leq \phi < 30°$ - $M = 0.1$
$30° \leq \phi$ - $M = 1$



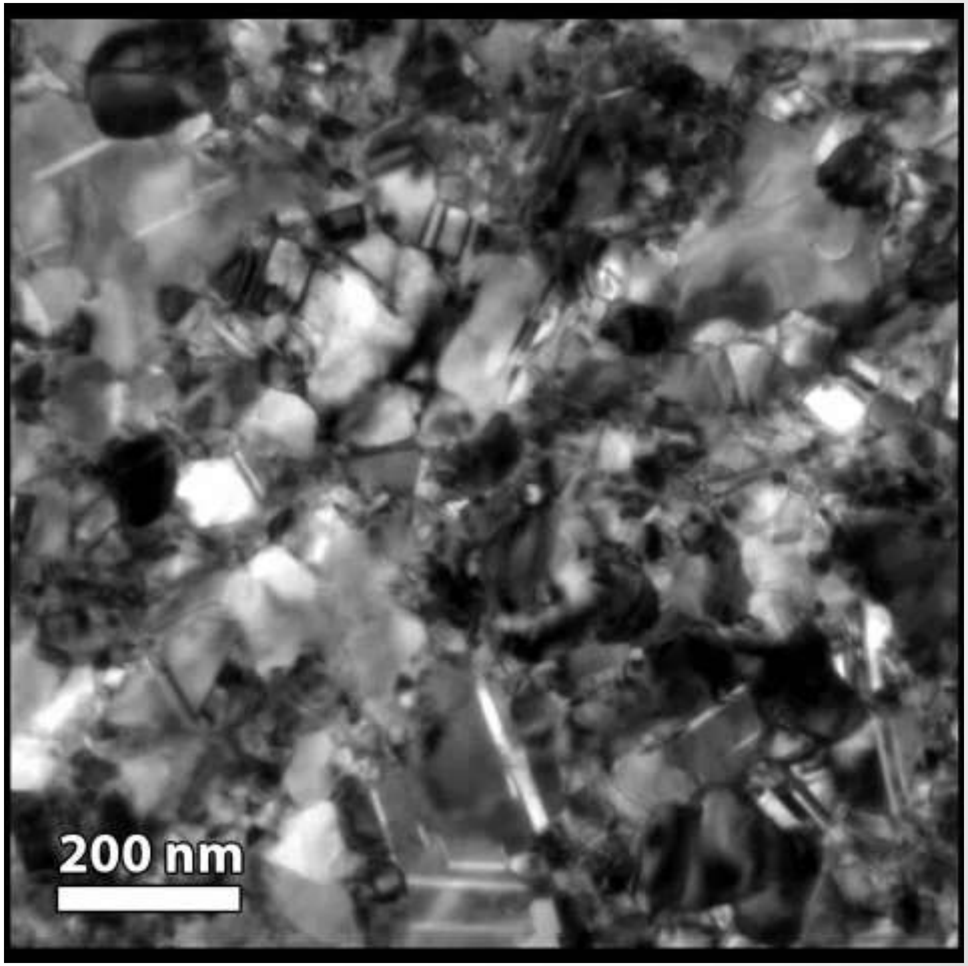
Implementation of heterogeneous boundary mobility

Future Directions

- Nature of Ion Interactions
  - Nuclear and electronic stopping
  - Point defects and defect clusters
- Dose rate
- Other materials and alloy systems
- Better informed GB mobility in model

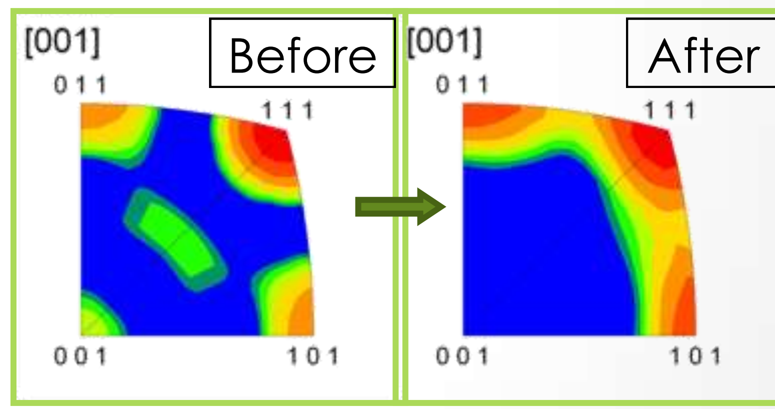


Homer, *et al*, JOM, 2014.



Summary

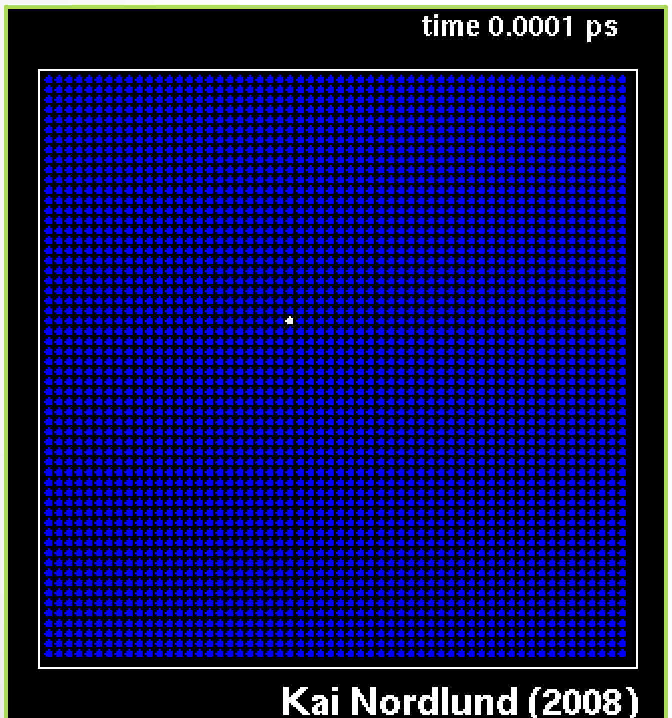
- TEM orientation mapping at various ion fluences
  - Analyzed and used as direct input for a phase field model
- Stable grains are characteristic of known low mobility grains
- Discrepancies between experimentally observed and modeled grain growth attributable to GB character



- Acknowledgements: A. Darbal (AppFive), D. Kaoumi (University of South Carolina), A. Leff (Drexel University), and B.L. Boyce, D.L. Buller, C. Gong, H. Lim, M.T. Marshall, and B.R. Muntifering (Sandia National Laboratories). This work was fully supported by the Division of Materials Science and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy.

Radiation-Solid Interactions

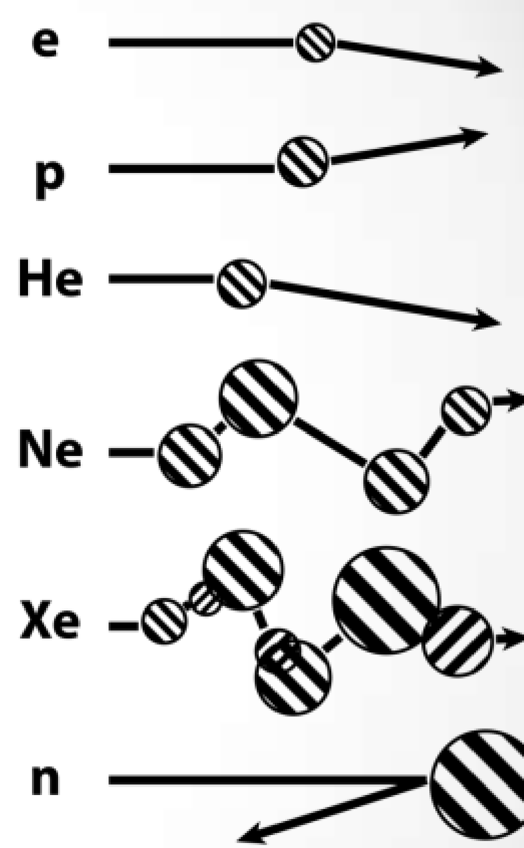
- Energetic ion displaces one or more target atoms
  - Frenkel (vacancy-interstitial) pair
  - Collision cascade
  - Nuclear and electronic interactions



10 keV Au in Au, *via* Wikimedia Commons.

Effective transient temperatures ~<u>thousand(s)</u> of K!

Affected volumes vary based on radiation species, energy, and target material.



Schematic recoil spectra for 1 MeV particles in Cu. Sizes represent recoil energies. After Averback, J Nucl Mater, 1994.

Highly temporally and spatially localized energy transfer drives microstructural change.

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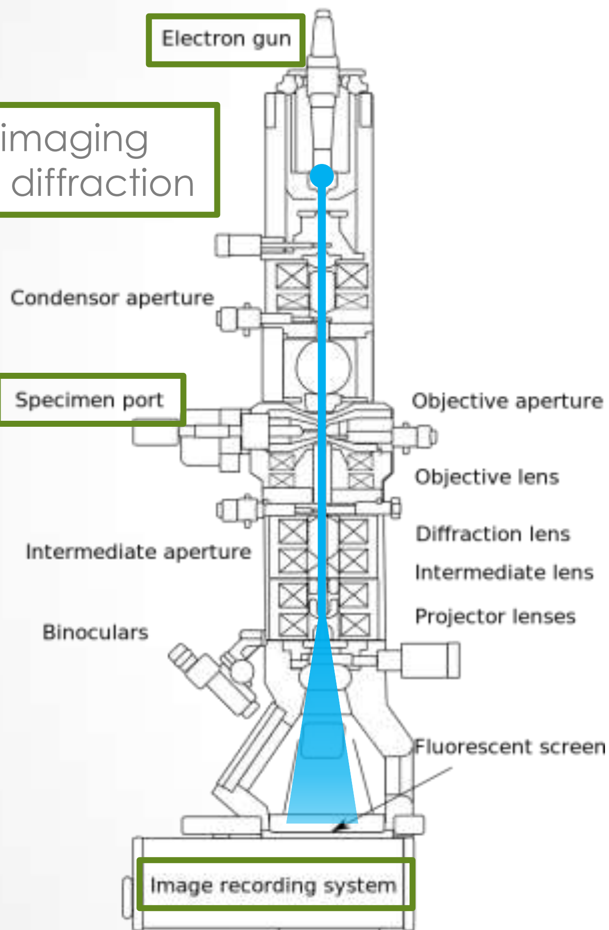
Sub-nm imaging
Electron diffraction



Gringer, 2009, *via* Wikimedia Commons.

Approach: Experimental

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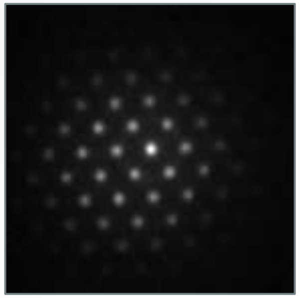
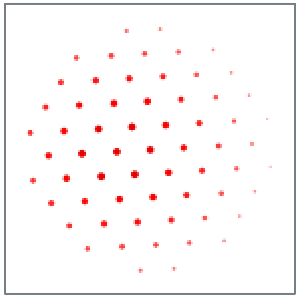
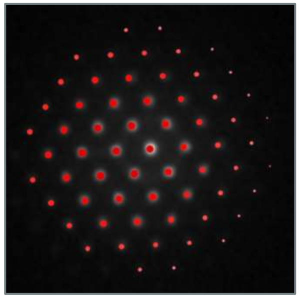


Experimental Pattern



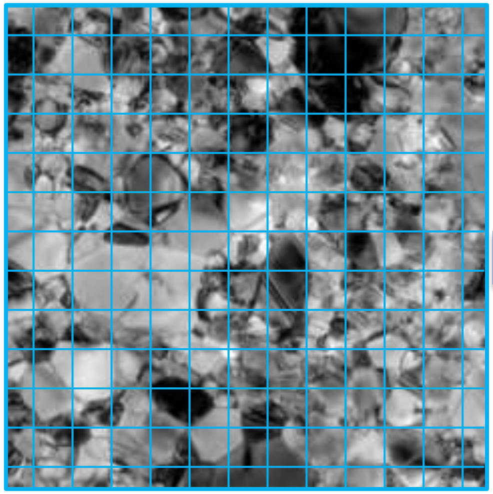
Theoretical Template

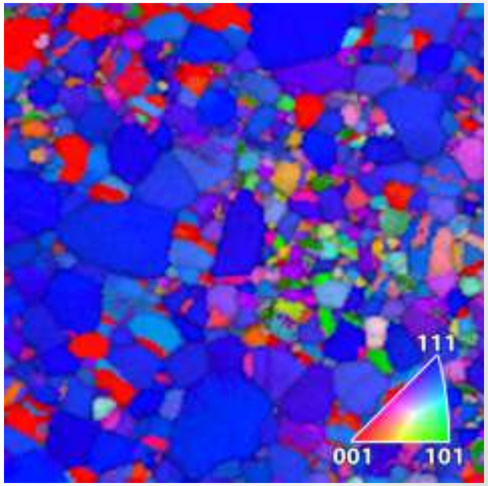


Template Matched

Point Mapped To IPF

- Automated diffraction orientation mapping
  - Point by point grid of orientations mapped
  - 5 nm resolution
- Analogous to EBSD

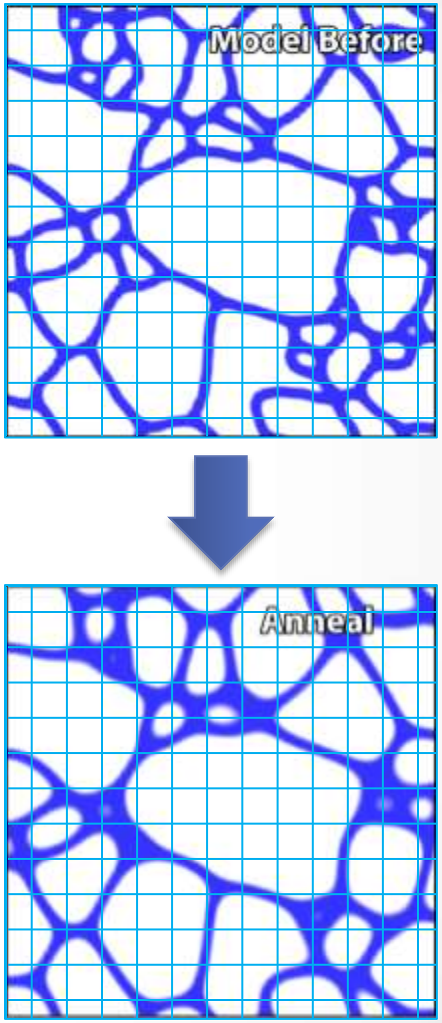




Point diffraction data

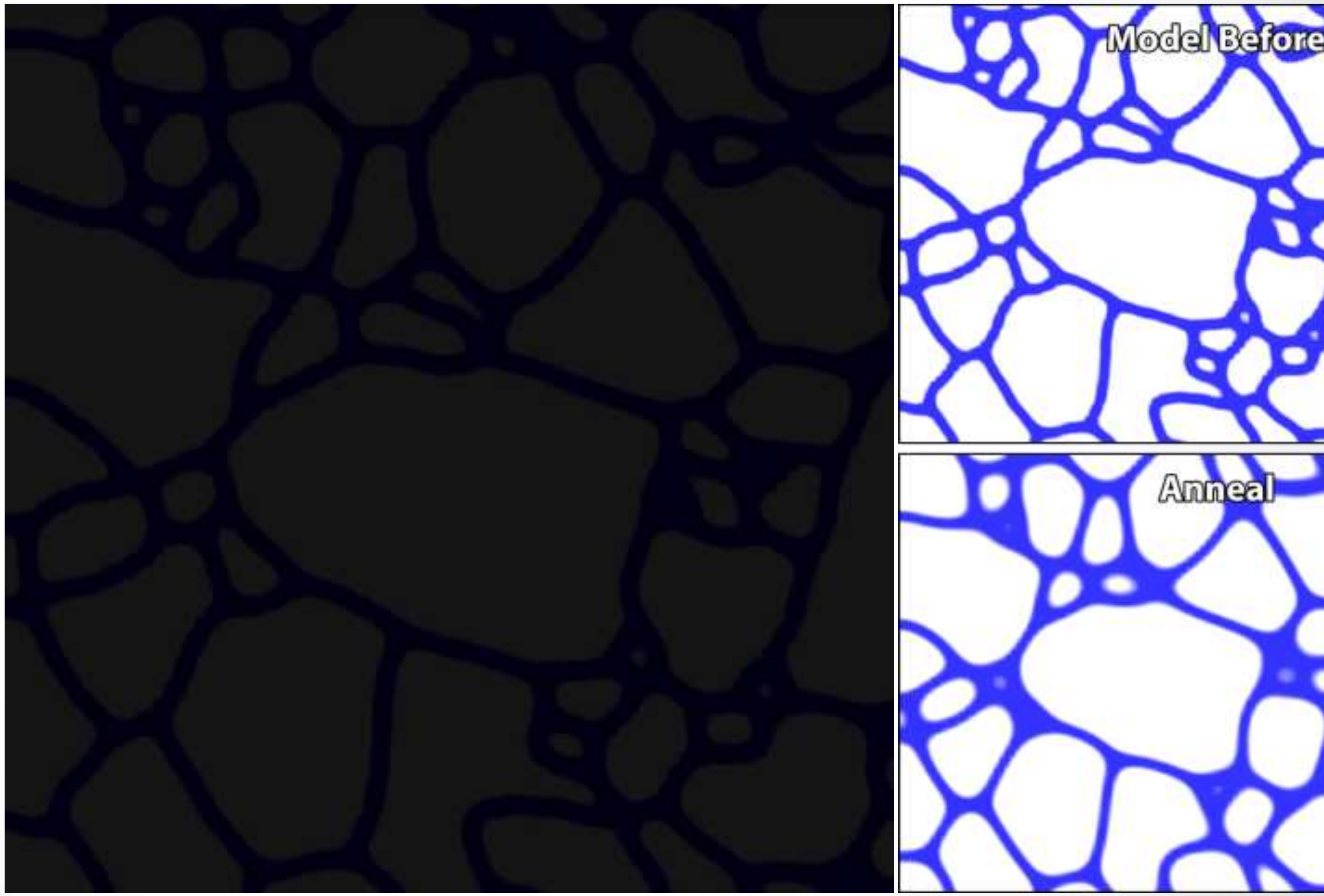
Approach: Modeling

- What is phase field modeling?
  - Mathematical model for solving interfacial problems, like solidification, growth, etc.
- Example grain growth model
  - Thermodynamic free energy function
    - $dF = d(\gamma A) = \gamma dA$ (γ: GB energy, A: GB area)
  - Model for kinetics
    - $V = M\gamma h$ (M: GB mobility, h: GB curvature)
  - Solve at each pixel for a predetermined timestep
- See Abdeljawad and Foiles, Acta Mater, 2015 for more information



Can directly use experimental maps as input structures, and then compare evolutions!

Simulated Anneal



Model Data Analysis

- During simulated annealing grain growth scales approximately with $T^{1/2}$
  - Expected for homogenous grain growth
- During simulated irradiation, grain growth scales with $T^{1/n}$, where $n \approx 3$
  - Initially faster, but stagnates sooner